

What makes an insulator different from a metal?

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Abstract. The insulating state of matter is characterized by the excitation spectrum, but also by qualitative features of the electronic ground state. The insulating ground wavefunction in fact: (i) displays vanishing dc conductivity; (ii) sustains macroscopic polarization; and (iii) is *localized*. The idea that the insulating state of matter is a consequence of electron localization was first proposed in 1964 by W. Kohn. I discuss here a novel definition of electron localization, rather different from Kohn’s, and deeply rooted in the modern theory of polarization. In fact the present approach links the two features (ii) and (iii) above, by means of essentially the same formalism. In the special case of an uncorrelated crystalline solid, the localization of the many-body insulating wavefunction is measured—according to our definition—by the spread of the Wannier orbitals; this spread diverges in the metallic limit. In the correlated case, the novel approach to localization is demonstrated by means of a two-band Hubbard model in one dimension, undergoing a transition from band insulator to Mott insulator.

INTRODUCTION

The present contribution, dealing with such a general issue as the difference between insulators and metals, may appear out of place at a workshop focussing on the “Fundamental Physics of Ferroelectrics”. But indeed, the present results are in a sense the ultimate developments of the theory of polarization [1–5] based on a Berry phase [6], which is crucial to the modern understanding of ferroelectrics [7]. The link between the present subject and polarization is simply stated: insulators sustain nontrivial bulk polarization, metals do not.

To the present purposes, materials are conveniently divided in only two classes: insulators and metals. We use here the terms in a loose sense as synonym of nonconducting and conducting: an insulator is distinguished from a metal by its vanishing conductivity at low temperature and low frequency. This qualitative difference in the dc conductivity must reflect a qualitative difference in the organization of the electrons in their ground state. So the question we are going to address is: is it possible to find a *pure ground state property* which discriminates between an insulator and a metal? Before proceeding to answer, let me discuss the

alternative phenomenological characterization of the insulating/metallic behavior: instead of making direct reference to the dc conductivity, we address macroscopic polarization.

Suppose we expose a finite macroscopic sample to an electric field, say inserting it in a charged capacitor. Then the induced macroscopic polarization is qualitatively different in metals and insulators. In the former materials polarization is trivial: universal, material-independent, due to surface phenomena only (screening by free carriers). Therefore polarization in metals is *not* a bulk phenomenon. The opposite is true for insulators: macroscopic polarization is a nontrivial, material-dependent, bulk phenomenon. We can therefore phenomenologically characterize an insulator, in very general terms, as a material whose ground wavefunction sustains a bulk macroscopic polarization whenever the electronic Hamiltonian is non centrosymmetric. From this definition it is clear that the modern theory of polarization, based on a Berry’s phase, can lead to a better understanding of the insulating state of matter.

This paper is organized as follows. First we briefly outline Kohn’s theory of the insulating state [8]. Then we address dipole and localization for a lone electron in a Born–von–Kàrmàn periodic box; subsequently, we apply similar ideas to an extended system of N electrons in a periodic box, addressing macroscopic polarization and electronic localization in the many-body case. We then show how this works for a crystalline system of independent electrons, and finally—following Ref. [9]—we demonstrate localization for a model correlated system displaying two different insulating phases. For the sake of simplicity, we explicitate here the relevant algebra only for the case of one-dimensional electrons. The generalization to three-dimensional electrons can be found in Refs. [10–12].

THE INSULATING STATE AND KOHN’S THEORY

Within any classical theory, the electronic responses of insulators and metals are qualitatively described by “bound” and “free” charges, respectively. Microscopic models for such charges are provided by the Lorentz theory (insulators) and by the Drude theory (metals). Within the former, each electron is tied (by an harmonic force) to a particular center; within the latter, electrons roam freely over macroscopic distances, hindered only by atomic scattering potentials. Therefore, from a purely classical model viewpoint, one explains the insulating/metallic behavior of a material by means of the localized/delocalized character of the electron distribution.

Switching to quantum mechanics, this clearcut character of the electron distribution is apparently lost. Textbooks typically explain the insulating/metallic behavior by means of band structure theory, focussing on the position of the Fermi level of the given material: either in an band gap (insulators), or across a band (metals). This picture is obviously correct, but very limited and somewhat misleading.

First of all, the band picture applies only to a crystalline material of independent

electrons: a very limited class of insulators indeed. Noncrystalline insulators do in fact exist, and the electron–electron interaction is a fact of nature: in some materials the insulating behavior is dominated by disorder (Anderson insulators), in some other materials the insulating behavior is dominated by electron correlation (Mott insulators). Further classes of insulators are also known, as *e.g.* excitonic insulators. Therefore, for a large number of insulators, the band picture is totally inadequate.

Second: even for a material where a band–structure description is adequate, the simple explanation of the insulating/metallic behavior focusses on the spectrum of the system, hence on the nature of the low lying electronic *excitations*. Instead, the qualitative difference in the dc conductivity at low temperature must reflect a qualitative difference in the organization of the electrons in their *ground state*. Such a difference is not evident in a band–structure picture: the occupied states are of the Bloch form both in insulators and in metals, and qualitatively rather similar (in particular those of simple metals and of simple semiconductors).

In a milestone paper published in 1964, Kohn was able to define the insulating state of matter in a way which in a sense is close to the classical picture. In fact he gave evidence that electron localization is the main feature determining the insulating behavior of a many–electron wavefunction [8], thus restoring the same basic distinction as in the classical picture: the key is how to define and to measure the degree of electronic localization, visualizing in a qualitative and quantitative way the peculiar organization of the electrons which is responsible for the insulating state of matter.

As previously stated, a superficial look indicates that electrons are roughly speaking equally delocalized in insulators and in metals. One needs therefore a sharp criterion which singles out the relevant character of the wavefunction. Kohn’s criterion is the following [8,13,12]: the many–electron wavefunction is localized if it breaks up into a sum of functions $\Psi = \sum_J \Psi_J$ which are localized in essentially disconnected regions \mathcal{R}_J of the configuration space. Any two such Ψ_J ’s have exponentially small overlap. Under such a localization hypothesis, Kohn proves that the dc conductivity vanishes.

DIPOLE AND LOCALIZATION FOR A SINGLE ELECTRON

The dipole moment of any *finite* N –electron system in its ground state is a simple and well defined quantity. Given the many–body wavefunction Ψ and the corresponding single–particle density $n(\mathbf{r})$ the electronic contribution to the dipole is:

$$\langle \mathbf{R} \rangle = \int d\mathbf{r} \, \mathbf{r} n(\mathbf{r}) = \langle \Psi | \hat{\mathbf{R}} | \Psi \rangle, \quad (1)$$

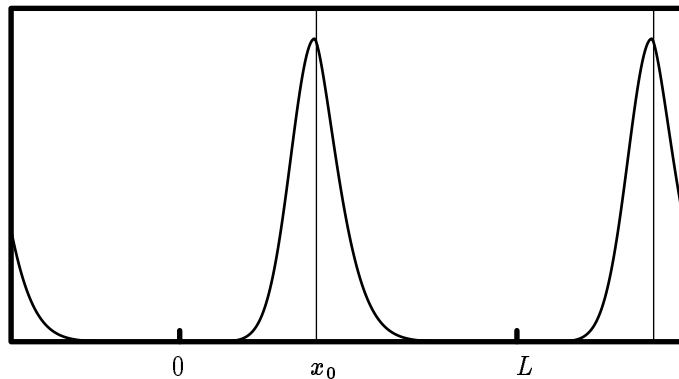


FIGURE 1. The distribution $|\psi(x)|^2$ of a single-particle orbital within periodic Born-von-Kàrmàn boundary conditions

where $\hat{\mathbf{R}} = \sum_{i=1}^N \mathbf{r}_i$. This looks very trivial, but we are exploiting here an essential fact: the ground wavefunction of any bound N -electron system is square-integrable and vanishes exponentially at infinity. Going at the very essence, we simplify matter at most and we consider in the present Section only a single electron in one dimension. The dipole (or equivalently the center) of the electronic distribution is then:

$$\langle x \rangle = \int_{-\infty}^{\infty} dx \, x |\psi(x)|^2, \quad (2)$$

where again we understand $\psi(x)$ as a square-integrable function over \mathbb{R} . This is not the way condensed matter theory works. Because of several good reasons, in either crystalline or disordered systems it is almost mandatory to assume BvK boundary conditions: the wavefunction $\psi(x)$ is periodic over a period L , large with respect to atomic dimensions.

Adopting a given choice for the boundary conditions is tantamount to defining the Hilbert space where our solutions of Schrödinger's equation live. By definition, an operator maps any vector of the given Hilbert space into another vector belonging to the same space: the multiplicative position operator x is therefore *not* a legitimate operator when BvK are adopted for the state vectors, while any periodic function of x is legitimate: this is the case *e.g.* of the nuclear potential acting on the electrons.

Suppose we have an electron distribution such as the one in Fig. 1. The main issue is then: how do we define the center of the distribution? Intuitively, the distribution appears to have a “center”, which however is defined only modulo the replica periodicity, and furthermore *cannot* be evaluated simply as in Eq. (2), precisely because of BvK.

Solutions to this and similar problems have been attempted several times: many incorrect papers—which will not be identified here—have been published over the years. The good solution has been found by Selloni *et al.* in 1987 by means of a very elegant and far-reaching formula [14]. According to them, the key quantity

for dealing with the position operator within BvK is the dimensionless complex number \mathfrak{z} , defined as:

$$\mathfrak{z} = \langle \psi | e^{i\frac{2\pi}{L}x} | \psi \rangle = \int_0^L dx e^{i\frac{2\pi}{L}x} |\psi(x)|^2, \quad (3)$$

whose modulus is no larger than 1. The most general electron density, such as the one depicted in Fig. 1, can always be written as a superposition of a function $n_{\text{loc}}(x)$, normalized over $(-\infty, \infty)$, and of its periodic replicas:

$$|\psi(x)|^2 = \sum_{m=-\infty}^{\infty} n_{\text{loc}}(x - x_0 - mL). \quad (4)$$

Both x_0 and $n_{\text{loc}}(x)$ have a large arbitrariness: we restrict it a little bit by imposing that x_0 is the center of the distribution, in the sense that $\int_{-\infty}^{\infty} dx x n_{\text{loc}}(x) = 0$. Using Eq. (4), \mathfrak{z} can be expressed in terms of the Fourier transform of n_{loc} as:

$$\mathfrak{z} = e^{i\frac{2\pi}{L}x_0} \tilde{n}_{\text{loc}}\left(-\frac{2\pi}{L}\right). \quad (5)$$

If the electron is localized in a region of space much smaller than L , its Fourier transform is smooth over reciprocal distances of the order of L^{-1} and can be expanded as:

$$\tilde{n}_{\text{loc}}\left(-\frac{2\pi}{L}\right) = 1 - \frac{1}{2} \left(\frac{2\pi}{L}\right)^2 \int_{-\infty}^{\infty} dx x^2 n_{\text{loc}}(x) + \mathcal{O}(L^{-3}). \quad (6)$$

A very natural definition of the center of a localized periodic distribution $|\psi(x)|^2$ is therefore provided by the phase of \mathfrak{z} as:

$$\langle x \rangle = \frac{L}{2\pi} \text{Im} \log \mathfrak{z}, \quad (7)$$

which is in fact the formula first proposed by Selloni *et al.* [14]. The expectation value $\langle x \rangle$ is defined modulo L , as expected since $|\psi(x)|^2$ is BvK periodic. It is also worth to observe that for an extremely delocalized state we have $|\psi(x)|^2 = 1/L$ and $\mathfrak{z} = 0$: hence the center of the distribution $\langle x \rangle$, according to Eq. (7), is ill-defined, as one would indeed expect.

So far, we have not specified which Hamiltonian we were addressing when discussing electron distributions $|\psi(x)|^2$ of the kind depicted in Fig. 1. It is however obvious to imagine that the wavefunction $\psi(x)$ is the eigenstate of a (periodically repeated) potential well of suitable shape. Suppose for a moment we are *not* adopting BvK boundary conditions, having thus only a genuinely isolated potential well. In this case the eigenstates can belong to two different classes: bound (localized) states, and scattering (delocalized) states. The distinction is a qualitatively

clearcut one, and can be stated in several ways. One of them is to consider the second cumulant moment, or spread:

$$\langle x^2 \rangle_c = \langle x^2 \rangle - \langle x \rangle^2 = \int_{-\infty}^{\infty} dx x^2 |\psi(x)|^2 - \left(\int_{-\infty}^{\infty} dx x |\psi(x)|^2 \right)^2, \quad (8)$$

which is finite for bound states and divergent (when using appropriate normalizations) for scattering ones. But if we study the same potential well within BvK, the qualitative distinction is lost: all states appear in a sense as “delocalized” since all wavefunctions $\psi(x)$ are periodic over the BvK period. And in fact the integrals in Eq. (8) become ill defined.

The main issues therefore are: How do we distinguish between localized and delocalized states within BvK? In case of a localized state, how we actually measure the amount of localization? In the literature, such issues have been previously addressed by means of the participation ratio [15]. The complex number \mathfrak{z} , whose phase provides the center of the distribution, Eq. (7), is our key to addressing localization: it is enough to consider its modulus. It has already been observed that $|\mathfrak{z}|$ is bounded between 0 and 1, and that $|\mathfrak{z}|$ equals zero for an extremely delocalized state with $|\psi(x)|^2 = 1/L$. If we take instead an extremely localized state, with $n_{\text{loc}}(x) = \delta(x)$, it is straightforward to get $|\mathfrak{z}| = 1$. It is therefore natural to measure localization by means of the negative of the logarithm of $|\mathfrak{z}|$: it is a nonnegative number, equal to zero in the case of extreme localization, and divergent in the case of extreme delocalization. A glance at Eq. (6) yields:

$$\log |\mathfrak{z}| \simeq -\frac{1}{2} \left(\frac{2\pi}{L} \right)^2 \int_{-\infty}^{\infty} dx x^2 n_{\text{loc}}(x), \quad (9)$$

hence a natural expression for measuring the actual spread within BvK is:

$$\langle x^2 \rangle_c = \langle x^2 \rangle - \langle x \rangle^2 = - \left(\frac{L}{2\pi} \right)^2 \log |\mathfrak{z}|^2. \quad (10)$$

Having in mind again the eigenstates of a potential well, we can study the expression in Eq. (10) as a function of L . For a localized state, the shape of $n_{\text{loc}}(x)$ can be taken as L -independent for large L , hence Eq. (10) goes to a finite limit, which is the “natural” spread of the distribution. Quite on the contrary, for a delocalized state the distribution is smeared all over the $(0, L)$ segment, preserving the norm over one period: therefore \mathfrak{z} goes to zero and the spread diverges in the large- L limit.

DIPOLE AND LOCALIZATION FOR MANY ELECTRONS

So much about the one-electron problem: we are now going to consider a finite density of electrons in the periodic box. To start with, irrelevant spin variables will

be neglected, and a system of spinless electrons in one dimension is considered. Even for a system of independent electrons, our approach takes a simple and compact form if a many-body formulation is adopted; BvK imposes periodicity in each electronic variable separately. Our interest is in studying a bulk system: N electrons in a segment of length L , where eventually the thermodynamic limit is taken: $L \rightarrow \infty$, $N \rightarrow \infty$, and $N/L = n_0$ constant.

We start defining the one-dimensional analogue of $\hat{\mathbf{R}}$ of Eq. (1), namely, the multiplicative operator $\hat{X} = \sum_{i=1}^N x_i$, and the complex number

$$\mathfrak{z}_N = \langle \Psi | e^{i\frac{2\pi}{L}\hat{X}} | \Psi \rangle. \quad (11)$$

It is obvious that the operator \hat{X} is ill-defined in our Hilbert space, while its complex exponential appearing in Eq. (11) is well defined. The main result of Ref. [4] is that the ground-state expectation value of the position operator is given by the analogue of Eq. (7), namely:

$$\langle X \rangle = \frac{L}{2\pi} \text{Im} \ln \mathfrak{z}_N, \quad (12)$$

a quantity defined modulo L as above.

The right-hand side of Eq. (12) is not simply the expectation value of an operator: it is the *phase* of it, converted into length units by the factor $L/(2\pi)$. This phase can be called a single-point Berry phase, for reasons explained elsewhere [16,10,11]. Furthermore, the main ingredient of Eq. (11) is the expectation value of the multiplicative operator $e^{i\frac{2\pi}{L}\hat{X}}$: it is important to realize that this is a genuine *many-body* operator. In general, one defines an operator to be one-body whenever it is the *sum* of N identical operators, acting on each electronic coordinate separately: for instance, the \hat{X} operator is such. In order to express the expectation value of a one-body operator the full many-body wavefunction is not needed: knowledge of the one-body reduced density matrix ρ is enough: I stress that, instead, the expectation value of $e^{i\frac{2\pi}{L}\hat{X}}$ over a correlated wavefunction *cannot* be expressed in terms of ρ , and knowledge of the N -electron wavefunction is explicitly needed. In the special case of a single-determinant, the N -particle wavefunction is uniquely determined by the one-body reduced density matrix ρ (which is the projector over the set of the occupied single-particle orbitals): therefore the expectation value $\langle X \rangle$, Eq. (12), is uniquely determined by ρ . But this is peculiar to uncorrelated wavefunctions only.

The expectation value $\langle X \rangle$ is extensive, as the dipole in Eq. (1). For the corresponding intensive quantity we borrow from Ref. [12] a useful notation:

$$\langle x \rangle_c = \langle X \rangle / N = \frac{L}{2\pi N} \text{Im} \ln \mathfrak{z}_N, \quad (13)$$

where the subscript means “cumulant”. The quantity $\langle x \rangle_c$ goes to a well defined thermodynamic limit, which is in fact proportional to the macroscopic polarization

of the system. This result is proved in Ref. [9]; its three dimensional generalization is discussed in Refs. [10–12].

We stress that nowhere have we assumed crystalline periodicity. Therefore our definition of $\langle x \rangle_c$ is very general: it applies to any condensed system, either ordered or disordered, either independent–electron or correlated. In the special case of a crystalline system, either interacting or noninteracting, the present approach can be shown equivalent to the previous formulations of polarization theory [1–4,10–12].

We are now ready to discuss electron localization in a condensed system: the present view is the one of Refs. [9,11], recently reexamined by Souza *et al.* [12], who also discuss its relationship to Kohn’s localization [8]. This view is based on the modulus of \mathfrak{z}_N , in full analogy with the previous Section about the single electron. We define therefore an intensive quantity, the second cumulant moment, by analogy with Eqs. (10) and (13):

$$\langle x^2 \rangle_c = -\frac{1}{N} \left(\frac{L}{2\pi} \right)^2 \log |\mathfrak{z}_N|^2, \quad (14)$$

where again the notation is borrowed from Ref. [12]. This second moment is a very meaningful measure of electron localization in the electronic ground wavefunction, and enjoys two important properties: (1) When applied to a crystalline system of independent electrons, we recover an important gauge–invariant quantity which controls the Marzari–Vanderbilt localization [17]; (2) Even for more general systems, correlated and/or disordered, $\langle x^2 \rangle_c$ assumes a finite value in insulators, and diverges in metals. Indeed in a metal the modulus of \mathfrak{z}_N goes to zero in such a way that its phase is ill defined, and hence macroscopic polarization is ill defined as well. We have emphasized throughout this paper that one of the main phenomenological features differentiating insulators from metals is that the former materials sustain a nontrivial bulk polarization, while the latter do not. The complex number \mathfrak{z}_N provides the key formal link between polarization and localization, via its phase and its modulus.

NONINTERACTING ELECTRONS

For independent electrons, we may write the many–body wavefunction Ψ as a Slater determinant of Bloch orbitals, but in the case of a metal not all the Bloch vectors in the reciprocal cell correspond to occupied orbitals: this fact is of overwhelming importance. We consider the simple case of one band in one dimension, whose Bloch vectors are illustrated in Fig. 2, imposing BvK boundary conditions over M cristal cells: $L = Ma$, where a is the lattice constant. We restore electron spin here: we get an insulator if the number of electrons N equals $2M$ (filled band, top sketch), and a metal if $N = M$ (half–filled band, bottom sketch). Both in the insulating and in the metallic case the N –electron wavefunction is a Slater determinant of size N , built of $N/2$ doubly occupied spatial orbitals. Following the

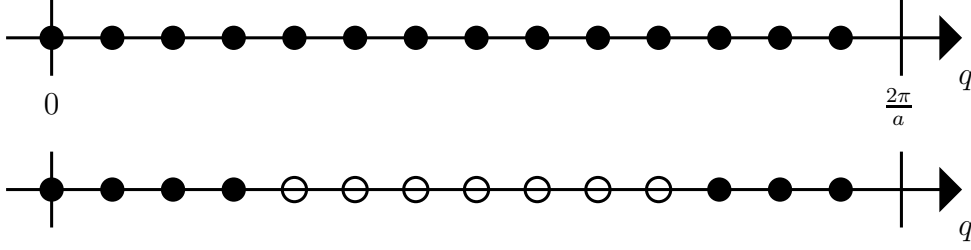


FIGURE 2. Discrete q vectors in the reciprocal cell in one dimension, where a BvK periodicity of $M = 14$ crystal cells has been chosen. Black circles correspond to occupied q 's, and empty circles to unoccupied ones. Top: insulator, with $N = 2M$ (filled band). Bottom: metal, with $N = M$ (half-filled band).

same algebra as in Refs. [4,10,11], the complex number \mathfrak{z}_N can be written in any case (insulator or metal) by means of the determinant of a matrix

$$\mathfrak{z}_N = (\det \mathcal{S})^2, \quad (15)$$

whose elements are

$$\mathcal{S}_{q_s, q_{s'}} = \frac{1}{a} \int dx \psi_{q_s}^*(x) \psi_{q_{s'}}(x) e^{i \frac{2\pi}{Ma} x}, \quad (16)$$

and these elements are nonzero whenever $s = s' + 1$.

In the insulating case, owing to complete filling, both s and s' run over all the M values: for any given s , there is always one (and only one) s' such that the matrix element in Eq. (16) is nonzero. That means that in any row of the \mathcal{S} matrix—whose size is $M \times M$ —there is one, and only one, nonvanishing element. Under these circumstances, the determinant factors as a product of M numbers:

$$\det \mathcal{S} = \prod_{s=0}^{M-1} \frac{1}{a} \int dx \psi_{q_{s+1}}^*(x) \psi_{q_s}(x) e^{i \frac{2\pi}{Ma} x}, \quad (17)$$

where the identity $\psi_{q_M}(x) \equiv \psi_{q_0}(x)$ is understood (periodic gauge). All the factors are nonvanishing, and the logarithm of \mathfrak{z}_N is therefore a finite number. It can be shown that the $N \rightarrow \infty$ limit of $\langle x^2 \rangle_c$ coincides with the spread of the optimally localized Wannier functions, as defined by Marzari and Vanderbilt [17].

The metallic case is very different. Since not all the q_s vectors are occupied, the indices s and s' run over a subset of the M values (Fig. 2): the matrix \mathcal{S} is of size $M/2 \times M/2$. There is one of the two q_s at the Fermi level, for which the integrals in Eq. (16) are all vanishing, for any *occupied* s' . Therefore the matrix \mathcal{S} has a row of zeros, and its determinant vanishes: its phase, and hence macroscopic polarization, is ill defined. The logarithm of \mathfrak{z}_N is formally $-\infty$, and the spread $\langle x^2 \rangle_c$ diverges to $+\infty$. This is what we expected for a metal; the nontrivial fact is that it diverges

even at finite N , while on general grounds we only expected it to diverge in the thermodynamic ($N \rightarrow \infty$) limit.

So far, the compact and elegant expression of Eq. (14) has been proved to be appropriate to discriminate between insulators and metals only for a crystalline systems of independent electrons. For the—much more interesting—general case of a correlated and/or disordered system, we *postulate* that Eq. (14) performs the same task. The postulate is based on the general argument—much stressed above—about macroscopic polarization: well defined in insulators, ill defined in metals (as a bulk property). The correctness of this postulate has been verified by Resta and Sorella [9] for a one-dimensional model of a correlated crystal. Work on a model disordered system is in progress. Other very interesting discussions about the physical meaning of $\langle x^2 \rangle_c$ and its relationships to the insulating/metallic character of the system can be found in a paper of Souza *et al.* [12].

LOCALIZATION IN A MODEL CORRELATED SYSTEM

We review here the very recent work of Resta and Sorella [9], where Eq. (14) is implemented for a one-dimensional two-band Hubbard model at half filling, intended to mimic an insulator having a mixed ionic/covalent character, and whose ground wavefunction is explicitly correlated. The macroscopic polarization of this model system was studied in Refs. [18,19]. To the present purpose, it is enough to study the centrosymmetric geometry: polarization is zero, the wavefunction is real, and the phase of \mathfrak{z}_N is either 0 or π .

The model has a very interesting behavior as a function of U : at small U it is a band insulator, while at a critical U_c undergoes a transition to a Mott-like insulating phase. In the centrosymmetric geometry, \mathfrak{z}_N is a real number, which changes sign at U_c . Its phase γ (*i.e.* the single-point Berry phase [16,10,11]) jumps therefore by π : it turns out that this occurrence is the main fact signalling the transition: the topological quantum number γ/π can be used as an order parameter to identify the two different phases of the system [20,21]. At low values of U our model is a band insulator, while above U_c is a Mott-like insulator. What happens to the second cumulant moment (squared localization length) $\langle x^2 \rangle_c$ as a function of U ?

The results are shown in Fig. 3 in terms of the dimensionless quantity

$$\mathcal{D}_N = -N \log |\mathfrak{z}_N|^2, \quad (18)$$

such that the squared localization length, Eq. (14) is;

$$\langle x^2 \rangle_c = \frac{1}{(2\pi n_0)^2} \lim_{N \rightarrow \infty} \mathcal{D}_N. \quad (19)$$

At $U = 0$ the system is noninteracting, and the squared localization length $\langle x^2 \rangle_c$ coincides with the second moment of the (optimally localized) Wannier function of the occupied band.

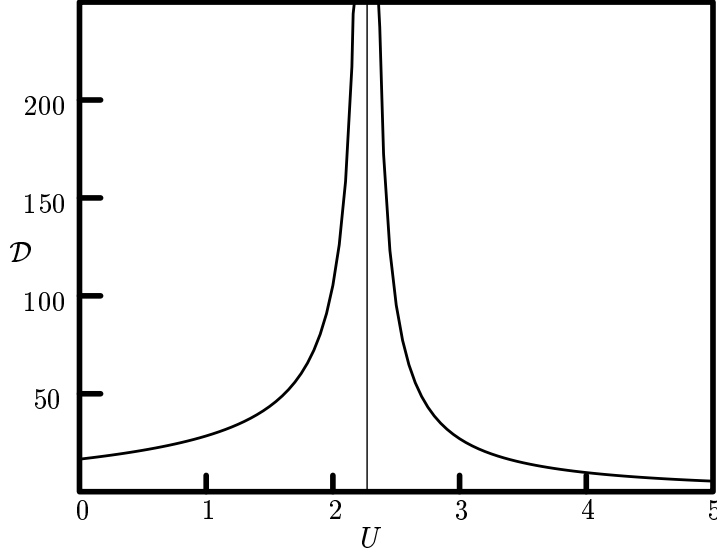


FIGURE 3. Dimensionless localization parameter, Eq. (18), as a function of U , after Ref. [9], where the effective value of N is 800. The divergence of the localization length at the Mott transition is perspicuous.

In the correlated case at $U \neq 0$ no Wannier analysis can be performed; yet $\langle x^2 \rangle_c$ maintains its role as a meaningful measure of the localization of the electronic wavefunction as a whole. The localization length increases with U below the transition, diverges at the transition point U_c , and becomes localized again in the highly correlated regime, where in fact $\langle x^2 \rangle_c$ decreases with increasing U . Since the localization length remains finite at all values of U different from U_c , the system is always insulating except at the transition point; the two insulating phases are topologically different and correspond to a qualitatively different organization of the electrons in the wavefunction [19].

What about the transition point? According to the previously stated viewpoint, the delocalized behavior implies a metallic character of the many-electron system. Notice that $\langle x^2 \rangle_c$ is a pure ground state property and apparently carries no information about the excitation spectrum of the system. Yet we have explicitly verified—by exploiting the metastability of the Lanczos algorithm—that at the critical U value there is indeed a level crossing. At the transition value U_c the ground state is twice degenerate and the lowest lying excitation (at constant N) has vanishing energy.

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